Dimethyl ethylmalonate 26717-67-9 | DTXSID70181214

Model F	Performance
---------	-------------

Model	Data	

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 198 °C

Global applicability domain: Inside

Local applicability domain index: 8.75e-01

Confidence level: 8.75e-01

Nearest Neighbors from the Training Set

Image not found

Propylene glycol diacetate

Measured: 191 Predicted: 198

Image not found

Diethyl propanedioate

Measured: 200 Predicted: 206

Image not found

Butanedioic acid, ethyl methyl

ester

Measured: 208 Predicted: 206

Image not found

1,3-Propanediol, diacetate

Measured: 210 Predicted: 206